



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:10 AM UTC

PDB ID : 9KK2 / pdb_00009kk2
EMDB ID : EMD-62382
Title : Cryo-EM structure of the Retron-Eco7 complex (state 5)
Authors : Ishikawa, J.; Yoneyama, K.; Yamashita, K.; Nishimasu, H.
Deposited on : 2024-11-12
Resolution : 2.58 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

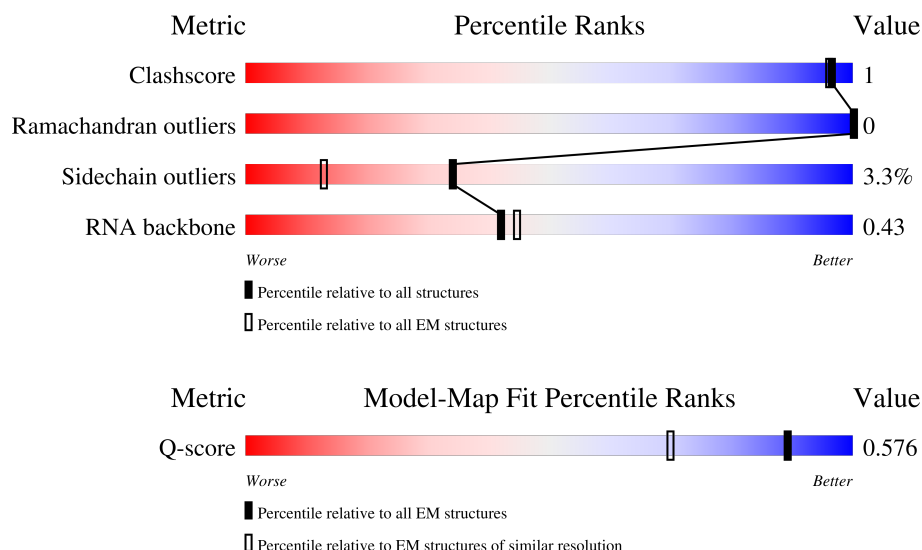
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7675 (2.08 - 3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	
1	K	322	
2	B	550	

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Mol	Chain	Length	Quality of chain
2	C	550	16%91%7%
2	D	550	14%88%9%
2	E	550	5%85%7%6%
3	F	266	76%21%
3	G	266	13%76%21%
4	H	146	18%7%72%
4	L	146	19%8%72%
5	I	77	83%12%5%
5	M	77	13%87%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28870 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	308	Total	C	N	O	S	0	0
			2473	1588	434	442	9		
1	K	308	Total	C	N	O	S	0	0
			2473	1588	434	442	9		

- Molecule 2 is a protein called AAA family ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	528	Total	C	N	O	S	2	0
			4256	2678	750	815	13		
2	C	535	Total	C	N	O	S	0	0
			4283	2694	752	824	13		
2	D	536	Total	C	N	O	S	2	0
			4307	2711	759	824	13		
2	E	516	Total	C	N	O	S	1	0
			4149	2618	728	791	12		

- Molecule 3 is a protein called TIGR02646 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	210	Total	C	N	O	S	0	0
			1701	1074	292	324	11		
3	G	210	Total	C	N	O	S	0	0
			1701	1074	292	324	11		

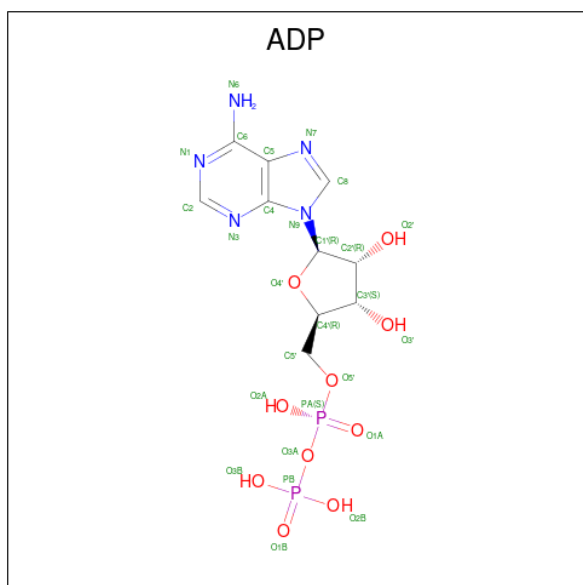
- Molecule 4 is a RNA chain called msrRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	41	Total	C	N	O	P	0	0
			869	389	149	290	41		
4	L	41	Total	C	N	O	P	0	0
			869	389	149	290	41		

- Molecule 5 is a DNA chain called msdDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	73	Total	C	N	O	P	0	0
			1501	711	285	432	73		
5	M	10	Total	C	N	O	P	0	0
			203	98	34	61	10		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	F	1	Total	Zn	0
			1	1	
7	G	1	Total	Zn	0
			1	1	

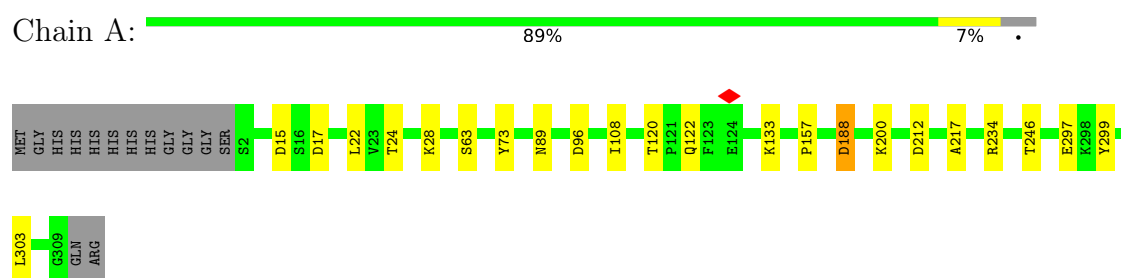
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	H	1	Total 1	Mg 1	0
8	L	1	Total 1	Mg 1	0

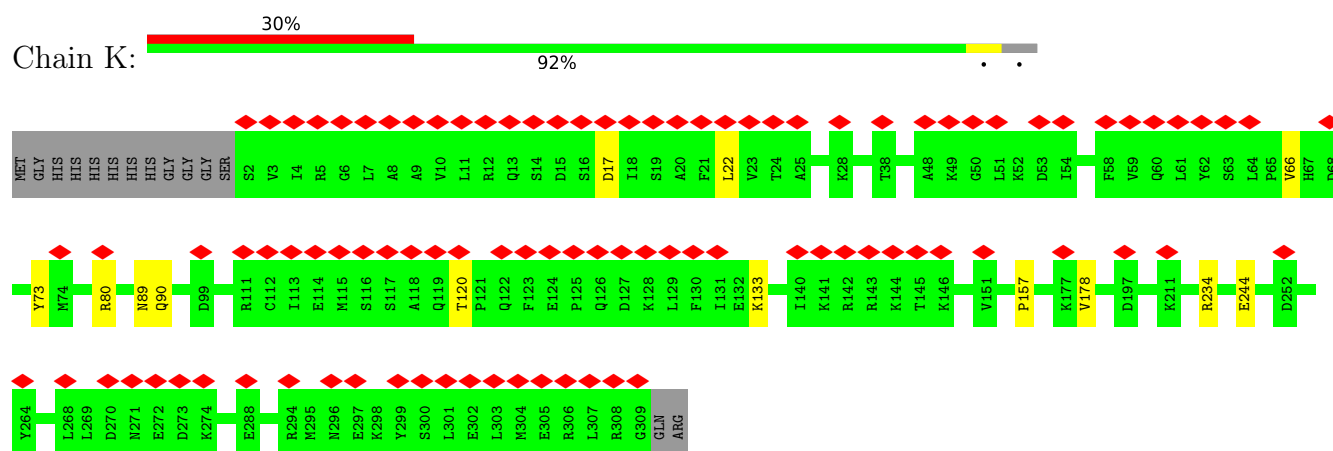
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

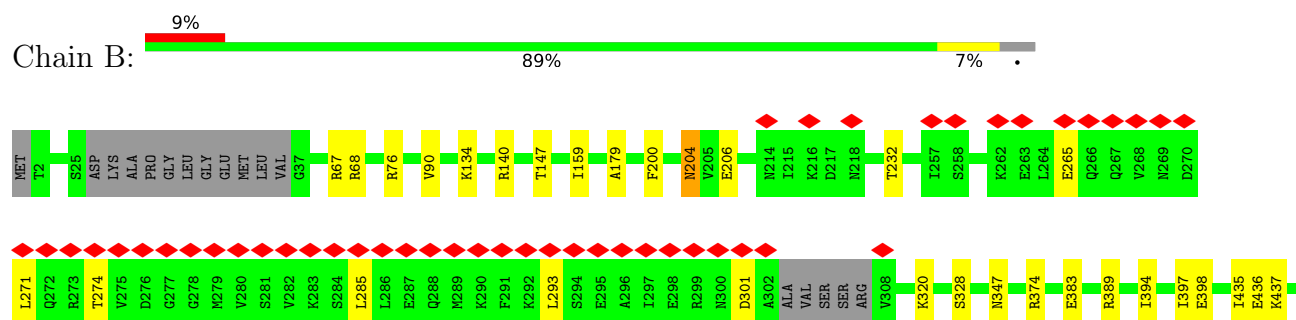
• Molecule 1: RNA-directed DNA polymerase

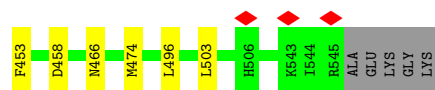


• Molecule 1: RNA-directed DNA polymerase

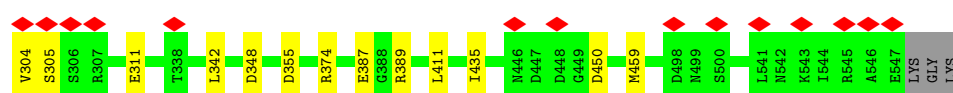
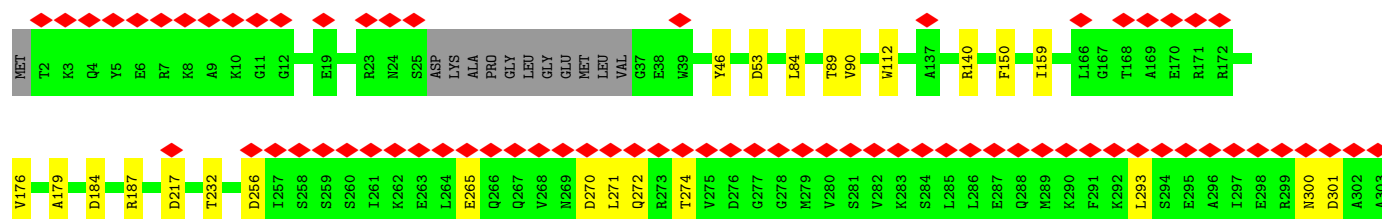
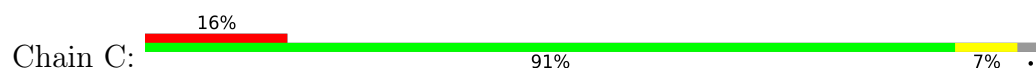


• Molecule 2: AAA family ATPase

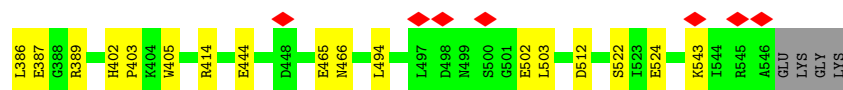
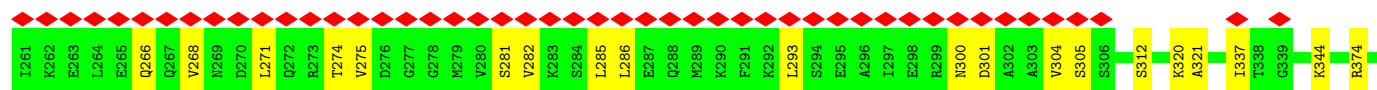
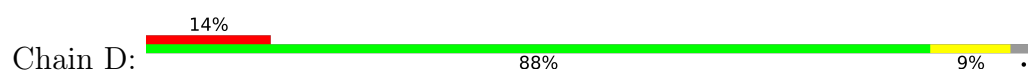




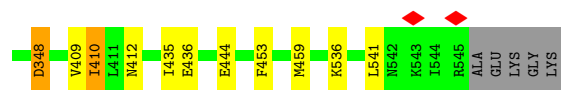
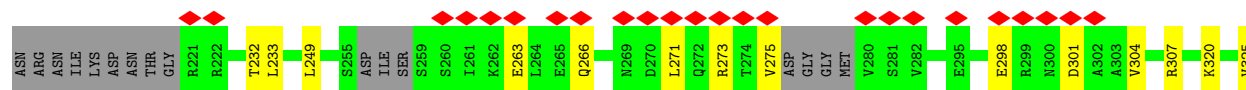
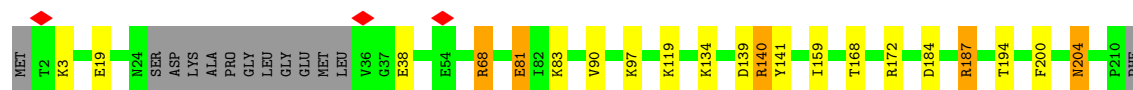
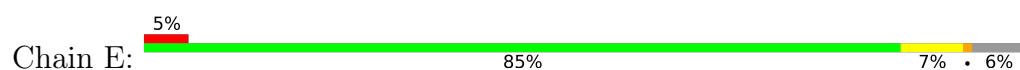
• Molecule 2: AAA family ATPase



• Molecule 2: AAA family ATPase



• Molecule 2: AAA family ATPase



• Molecule 3: TIGR02646 family protein

[illegible]

Diagram illustrating the structure of a 128-bit vector V . The vector is divided into three parts: a 64-bit gray section (DC, DA, DA, DC, DC, DC, DC, DT), a 32-bit green section (T68, T71, C77), and a 32-bit red section. Red diamonds are placed above the T68 and T71 labels.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	180392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.403	Depositor
Minimum map value	-0.787	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.996, 0.996, 0.996	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/2526	1.13	5/3408 (0.1%)
1	K	0.59	0/2526	1.11	3/3408 (0.1%)
2	B	0.64	0/4327	1.15	7/5834 (0.1%)
2	C	0.62	0/4355	1.14	8/5875 (0.1%)
2	D	0.64	0/4383	1.16	9/5914 (0.2%)
2	E	0.63	0/4221	1.15	14/5692 (0.2%)
3	F	0.68	0/1740	1.31	3/2352 (0.1%)
3	G	0.69	0/1740	1.34	4/2352 (0.2%)
4	H	0.59	0/970	1.14	8/1508 (0.5%)
4	L	0.65	0/970	0.92	3/1508 (0.2%)
5	I	0.40	0/1686	1.13	8/2600 (0.3%)
5	M	0.42	0/226	0.99	0/346
All	All	0.62	0/29670	1.15	72/40797 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	453	PHE	CA-CB-CG	10.38	124.18	113.80
4	H	42	A	O3'-P-O5'	-9.77	89.35	104.00
2	E	453	PHE	CA-CB-CG	9.52	123.31	113.80
3	G	126	VAL	N-CA-CB	9.49	121.06	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	45	U	O3'-P-O5'	-9.35	89.98	104.00
1	K	17	ASP	CA-CB-CG	8.64	121.24	112.60
1	A	17	ASP	CA-CB-CG	8.29	120.89	112.60
1	A	188	ASP	CA-CB-CG	8.19	120.79	112.60
2	E	348	ASP	CA-CB-CG	8.02	120.62	112.60
4	L	42	A	O3'-P-O5'	-7.89	92.16	104.00
2	E	301	ASP	CA-CB-CG	7.84	120.44	112.60
2	C	53	ASP	CA-CB-CG	7.65	120.25	112.60
4	H	26	U	O3'-P-O5'	-7.57	92.65	104.00
4	H	29	U	O3'-P-O5'	-7.26	93.11	104.00
5	I	13	DA	O3'-P-O5'	-6.94	93.59	104.00
4	H	47	A	O3'-P-O5'	-6.93	93.61	104.00
4	H	48	U	O3'-P-O5'	-6.79	93.82	104.00
2	D	268	VAL	N-CA-CB	6.60	120.48	110.58
2	C	355	ASP	CA-CB-CG	6.49	119.09	112.60
2	C	374	ARG	CD-NE-CZ	6.33	133.27	124.40
2	E	409	VAL	N-CA-CB	6.18	117.78	110.55
5	I	44	DG	O3'-P-O5'	-6.10	94.85	104.00
3	G	199	ASP	CA-CB-CG	6.09	118.69	112.60
3	F	199	ASP	CA-CB-CG	6.07	118.67	112.60
4	L	48	U	O3'-P-O5'	-6.07	94.90	104.00
2	D	163	ARG	NE-CZ-NH2	6.06	124.65	119.20
5	I	20	DG	O3'-P-O5'	-5.95	95.07	104.00
2	E	140	ARG	NE-CZ-NH2	5.95	124.55	119.20
2	B	389	ARG	CB-CA-C	-5.90	99.51	109.83
3	F	180	PHE	CA-CB-CG	5.88	119.68	113.80
3	G	180	PHE	CA-CB-CG	5.79	119.59	113.80
1	K	244	GLU	CB-CG-CD	5.73	122.34	112.60
4	H	46	U	C1'-C2'-O2'	-5.70	103.25	111.80
4	H	23	G	O3'-P-O5'	-5.69	95.46	104.00
2	B	374	ARG	CD-NE-CZ	5.69	132.37	124.40
2	E	187	ARG	CD-NE-CZ	5.65	132.31	124.40
2	B	383	GLU	N-CA-CB	5.56	118.08	110.01
2	E	536	LYS	CB-CA-C	-5.54	101.95	110.81
1	A	212	ASP	CA-CB-CG	5.53	118.13	112.60
5	I	74	DG	O3'-P-O5'	-5.46	95.81	104.00
2	D	238	ARG	NE-CZ-NH2	5.45	124.11	119.20
5	I	35	DA	O3'-P-O5'	-5.43	95.86	104.00
2	D	387	GLU	CB-CG-CD	5.42	121.82	112.60
1	K	90	GLN	N-CA-CB	5.41	118.45	110.33
5	I	49	DG	O3'-P-O5'	-5.38	95.94	104.00
5	I	31	DG	O3'-P-O5'	-5.36	95.96	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	168	THR	CA-CB-OG1	-5.28	101.68	109.60
2	C	387	GLU	CB-CG-CD	5.26	121.55	112.60
4	L	47	A	O3'-P-O5'	-5.25	96.12	104.00
2	E	139	ASP	CA-CB-CG	5.25	117.85	112.60
2	D	217	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	301	ASP	CA-CB-CG	5.21	117.81	112.60
2	D	374	ARG	CD-NE-CZ	5.19	131.66	124.40
2	D	275	VAL	N-CA-CB	5.18	118.36	110.58
2	C	389	ARG	CB-CA-C	-5.18	100.77	109.83
2	C	256	ASP	CA-CB-CG	5.17	117.77	112.60
3	G	105	ASP	CA-CB-CG	5.16	117.76	112.60
2	B	68	ARG	CD-NE-CZ	5.16	131.63	124.40
2	D	389	ARG	CB-CA-C	-5.16	100.81	109.83
1	A	200	LYS	CB-CA-C	-5.14	101.12	110.63
1	A	15	ASP	CA-CB-CG	5.13	117.73	112.60
2	E	307	ARG	CD-NE-CZ	5.12	131.57	124.40
5	I	22	DA	O3'-P-O5'	-5.12	96.32	104.00
2	E	204	ASN	CA-CB-CG	5.10	117.70	112.60
2	E	536	LYS	CA-CB-CG	5.10	124.30	114.10
2	D	414	ARG	CB-CG-CD	5.10	123.02	111.30
2	E	536	LYS	N-CA-CB	5.09	117.53	109.94
2	B	76	ARG	NE-CZ-NH2	5.08	123.78	119.20
2	E	444	GLU	CB-CG-CD	5.05	121.19	112.60
2	C	348	ASP	CA-CB-CG	5.04	117.64	112.60
3	F	105	ASP	CA-CB-CG	5.04	117.64	112.60
2	C	311	GLU	CB-CG-CD	5.02	121.14	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	217	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2473	0	2532	6	0
1	K	2473	0	2532	4	0
2	B	4256	0	4250	8	0
2	C	4283	0	4275	10	0
2	D	4307	0	4308	8	0
2	E	4149	0	4155	11	0
3	F	1701	0	1631	0	0
3	G	1701	0	1631	0	0
4	H	869	0	438	0	0
4	L	869	0	438	0	0
5	I	1501	0	818	1	0
5	M	203	0	115	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	E	27	0	12	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
8	H	1	0	0	0	0
8	L	1	0	0	0	0
All	All	28870	0	27159	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:ASP:OD1	2:C:187:ARG:NH1	2.24	0.67
2:E:194:THR:OG1	2:E:304:VAL:O	2.17	0.63
1:K:89:ASN:O	1:K:234:ARG:NH2	2.32	0.62
2:B:90:VAL:HG21	2:B:435:ILE:HD13	1.81	0.61
2:C:301:ASP:O	2:C:305:SER:N	2.31	0.61
2:E:90:VAL:HG21	2:E:435:ILE:HD13	1.83	0.61
2:C:265:GLU:HG3	2:C:293:LEU:HD11	1.85	0.59
2:C:90:VAL:HG21	2:C:435:ILE:HD13	1.84	0.58
2:E:184:ASP:OD1	2:E:187:ARG:NH1	2.33	0.57
2:E:200:PHE:O	2:E:232:THR:OG1	2.22	0.57
2:B:265:GLU:HG3	2:B:293:LEU:HD11	1.87	0.55
1:K:73:TYR:CG	1:K:157:PRO:HB3	2.44	0.52
2:C:159:ILE:CD1	2:C:179:ALA:HB2	2.41	0.50
1:K:22:LEU:O	1:K:133:LYS:HD3	2.12	0.50
2:C:84:LEU:HD23	2:C:89:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:300:ASN:O	2:C:304:VAL:HG23	2.13	0.49
1:A:89:ASN:O	1:A:234:ARG:NH1	2.46	0.49
2:D:84:LEU:HD23	2:D:89:THR:HG21	1.96	0.48
2:B:134:LYS:O	2:B:140:ARG:NH2	2.48	0.47
2:E:119:LYS:NZ	5:I:42:DT:OP1	2.47	0.47
2:C:270:ASP:OD2	2:D:281:SER:OG	2.32	0.47
2:E:325:VAL:HA	2:E:412:ASN:HB3	1.96	0.46
1:A:22:LEU:O	1:A:133:LYS:HD3	2.16	0.46
1:A:108:ILE:HD11	1:A:217:ALA:HB1	1.97	0.46
2:C:112:TRP:CZ3	2:C:176:VAL:HG21	2.51	0.46
2:D:301:ASP:O	2:D:305:SER:N	2.40	0.46
2:E:134:LYS:O	2:E:140:ARG:NH1	2.48	0.46
1:A:73:TYR:CG	1:A:157:PRO:HB3	2.51	0.46
2:E:68:ARG:NE	2:E:81:GLU:OE2	2.50	0.45
2:B:394:ILE:HG21	2:B:397:ILE:HD12	1.99	0.45
1:A:24:THR:OG1	1:A:28:LYS:NZ	2.49	0.44
1:K:73:TYR:CD2	1:K:157:PRO:HB3	2.52	0.44
2:B:204:ASN:ND2	2:B:206:GLU:HB2	2.32	0.44
2:E:141:TYR:CD1	2:E:172:ARG:HD2	2.54	0.43
1:A:299:TYR:HB3	1:A:303:LEU:HD23	2.01	0.42
2:D:402[B]:HIS:CE1	2:D:405:TRP:CD1	3.07	0.42
2:D:300:ASN:O	2:D:304:VAL:HG23	2.19	0.42
2:D:321:ALA:HB2	2:D:386:LEU:HD11	2.02	0.42
2:B:328:SER:HB2	2:B:347:ASN:OD1	2.20	0.42
2:D:522:SER:OG	2:D:524:GLU:OE1	2.38	0.42
2:E:232:THR:HG23	2:E:233:LEU:HG	2.02	0.41
2:B:159:ILE:CD1	2:B:179:ALA:HB2	2.51	0.41
2:D:200:PHE:O	2:D:232:THR:OG1	2.36	0.41
2:E:410:ILE:HD13	2:E:435:ILE:HD11	2.02	0.41
2:C:46:TYR:OH	2:C:150:PHE:O	2.30	0.41
2:B:200:PHE:O	2:B:232:THR:OG1	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/322 (95%)	303 (99%)	3 (1%)	0	100	100
1	K	306/322 (95%)	301 (98%)	5 (2%)	0	100	100
2	B	524/550 (95%)	510 (97%)	14 (3%)	0	100	100
2	C	531/550 (96%)	520 (98%)	11 (2%)	0	100	100
2	D	534/550 (97%)	524 (98%)	10 (2%)	0	100	100
2	E	507/550 (92%)	497 (98%)	10 (2%)	0	100	100
3	F	208/266 (78%)	194 (93%)	14 (7%)	0	100	100
3	G	208/266 (78%)	194 (93%)	14 (7%)	0	100	100
All	All	3124/3376 (92%)	3043 (97%)	81 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/279 (96%)	262 (97%)	7 (3%)	40	66
1	K	269/279 (96%)	265 (98%)	4 (2%)	57	78
2	B	475/489 (97%)	459 (97%)	16 (3%)	32	58
2	C	478/489 (98%)	469 (98%)	9 (2%)	50	73
2	D	481/489 (98%)	454 (94%)	27 (6%)	19	38
2	E	464/489 (95%)	442 (95%)	22 (5%)	23	46
3	F	179/216 (83%)	175 (98%)	4 (2%)	45	70
3	G	179/216 (83%)	174 (97%)	5 (3%)	38	64
All	All	2794/2946 (95%)	2700 (97%)	94 (3%)	34	58

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	96	ASP
1	A	120	THR
1	A	122	GLN
1	A	188	ASP
1	A	246	THR
1	A	297	GLU
2	B	67[A]	ARG
2	B	67[B]	ARG
2	B	147	THR
2	B	204	ASN
2	B	271	LEU
2	B	274	THR
2	B	285	LEU
2	B	320	LYS
2	B	398	GLU
2	B	436	GLU
2	B	437	LYS
2	B	458	ASP
2	B	466	ASN
2	B	474	MET
2	B	496	LEU
2	B	503	LEU
2	C	140	ARG
2	C	232	THR
2	C	271	LEU
2	C	272	GLN
2	C	274	THR
2	C	342	LEU
2	C	411	LEU
2	C	450	ASP
2	C	459	MET
2	D	35	LEU
2	D	41	GLU
2	D	72	LYS
2	D	119	LYS
2	D	159	ILE
2	D	172	ARG
2	D	219	THR
2	D	266	GLN
2	D	271	LEU
2	D	274	THR
2	D	282	VAL

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Mol	Chain	Res	Type
2	D	285	LEU
2	D	286	LEU
2	D	293	LEU
2	D	312	SER
2	D	320	LYS
2	D	337	ILE
2	D	344	LYS
2	D	403	PRO
2	D	444	GLU
2	D	465	GLU
2	D	466	ASN
2	D	494	LEU
2	D	502	GLU
2	D	503	LEU
2	D	512	ASP
2	D	543	LYS
2	E	3	LYS
2	E	19	GLU
2	E	38	GLU
2	E	68	ARG
2	E	81	GLU
2	E	83	LYS
2	E	97	LYS
2	E	159	ILE
2	E	204	ASN
2	E	249	LEU
2	E	263	GLU
2	E	266	GLN
2	E	271	LEU
2	E	273	ARG
2	E	275	VAL
2	E	298	GLU
2	E	320	LYS
2	E	348	ASP
2	E	410	ILE
2	E	436	GLU
2	E	459	MET
2	E	541	LEU
3	F	1	MET
3	F	11	GLU
3	F	28	GLN
3	F	161	THR

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Mol	Chain	Res	Type
3	G	1	MET
3	G	11	GLU
3	G	28	GLN
3	G	126	VAL
3	G	161	THR
1	K	66	VAL
1	K	80	ARG
1	K	120	THR
1	K	178	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
2	B	116	ASN
2	B	204	ASN
2	B	214	ASN
2	B	267	GLN
2	B	466	ASN
2	B	499	ASN
2	B	535	ASN
2	B	542	ASN
2	C	241	HIS
2	C	267	GLN
2	C	466	ASN
2	C	499	ASN
2	D	125	GLN
2	D	135	ASN
2	D	466	ASN
2	E	51	HIS
2	E	95	ASN
2	E	116	ASN
2	E	272	GLN
2	E	300	ASN
2	E	361	GLN
2	E	451	GLN
2	E	466	ASN
2	E	499	ASN
3	G	57	HIS
3	G	164	GLN
1	K	46	GLN
1	K	221	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	H	40/146 (27%)	9 (22%)	2 (5%)
4	L	40/146 (27%)	10 (25%)	4 (10%)
All	All	80/292 (27%)	19 (23%)	6 (7%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	H	27	G
4	H	28	A
4	H	29	U
4	H	37	A
4	H	40	C
4	H	42	A
4	H	43	A
4	H	44	C
4	H	48	U
4	L	24	G
4	L	28	A
4	L	29	U
4	L	40	C
4	L	42	A
4	L	43	A
4	L	44	C
4	L	48	U
4	L	49	U
4	L	50	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	H	46	U
4	H	48	U
4	L	41	U
4	L	43	A
4	L	46	U
4	L	48	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ADP	B	601	-	28,29,29	0.58	0	43,45,45	0.82	2 (4%)
6	ADP	E	601	-	28,29,29	0.45	0	43,45,45	0.64	0
6	ADP	C	601	-	28,29,29	0.41	0	43,45,45	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	B	601	-	-	4/16/32/32	0/3/3/3
6	ADP	E	601	-	-	2/16/32/32	0/3/3/3
6	ADP	C	601	-	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	ADP	O2A-PA-O3A	2.17	113.15	107.27
6	B	601	ADP	O3'-C3'-C4'	-2.01	105.31	111.08

There are no chirality outliers.

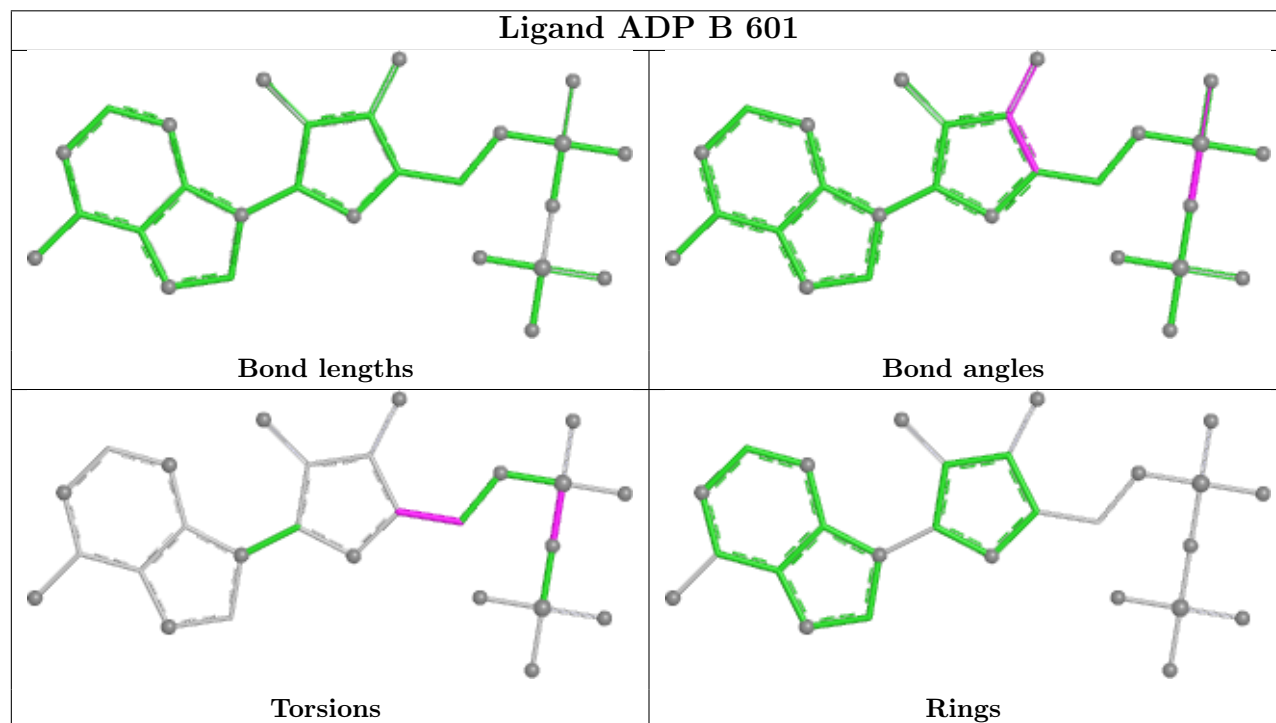
All (8) torsion outliers are listed below:

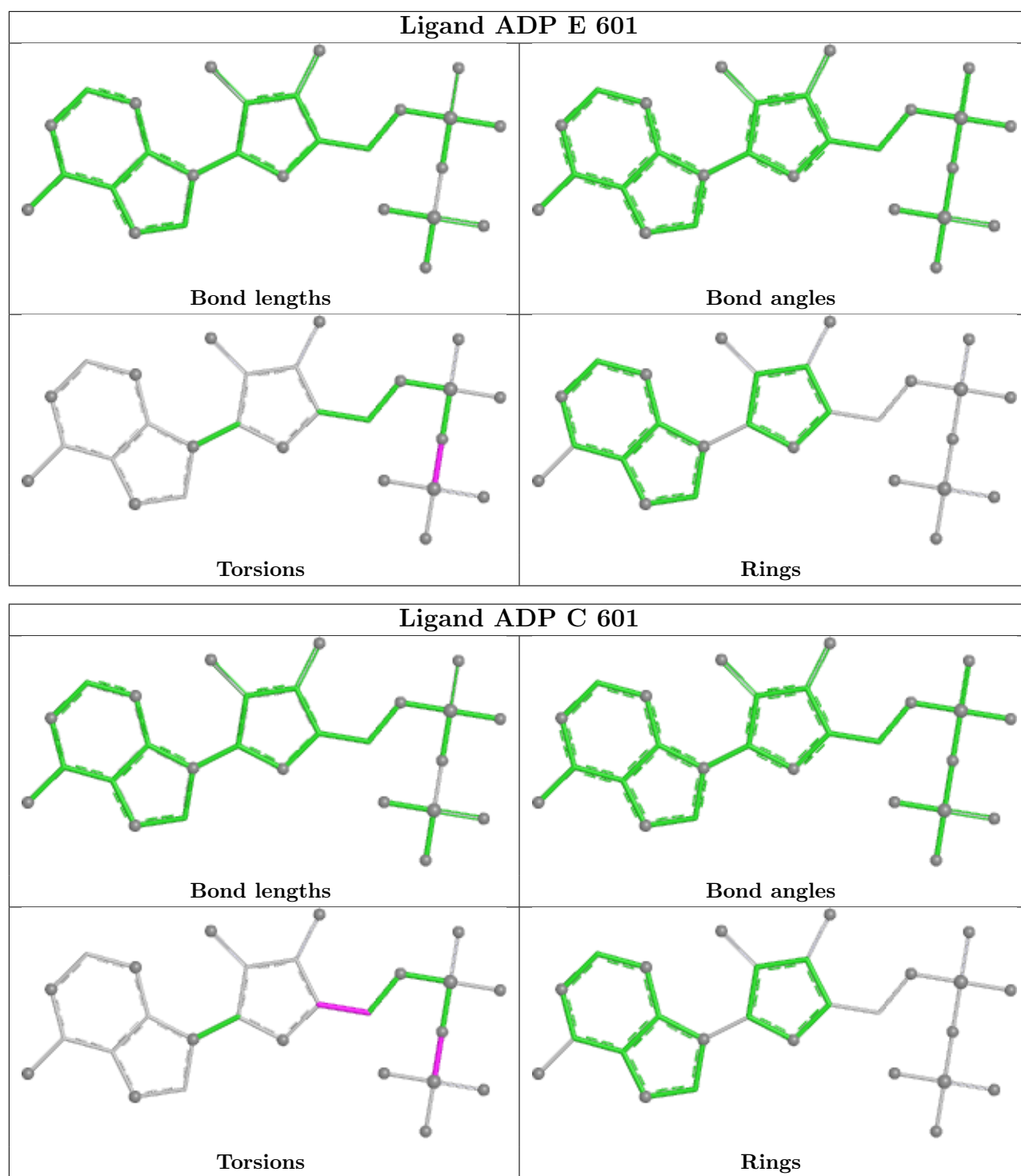
Mol	Chain	Res	Type	Atoms
6	C	601	ADP	PA-O3A-PB-O2B
6	E	601	ADP	PA-O3A-PB-O2B
6	B	601	ADP	O4'-C4'-C5'-O5'
6	B	601	ADP	C3'-C4'-C5'-O5'
6	C	601	ADP	C3'-C4'-C5'-O5'
6	B	601	ADP	PB-O3A-PA-O2A
6	B	601	ADP	PB-O3A-PA-O1A
6	E	601	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

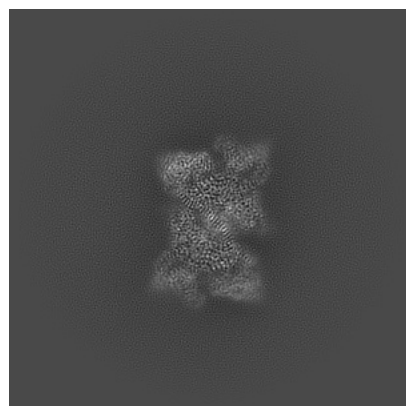
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62382. These allow visual inspection of the internal detail of the map and identification of artifacts.

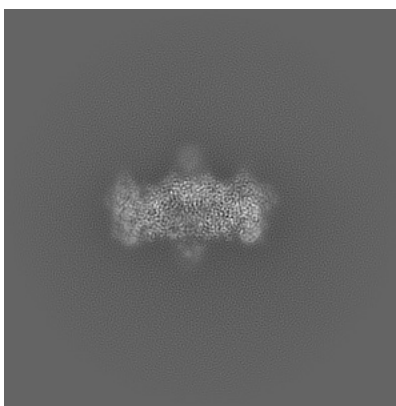
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

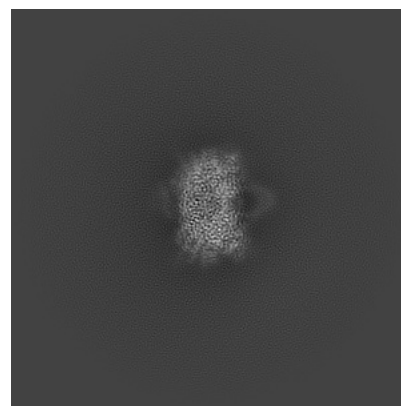
6.1.1 Primary map



X

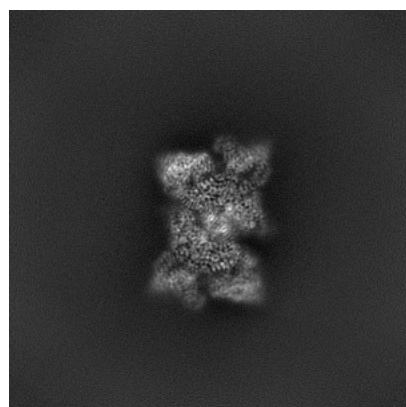


Y

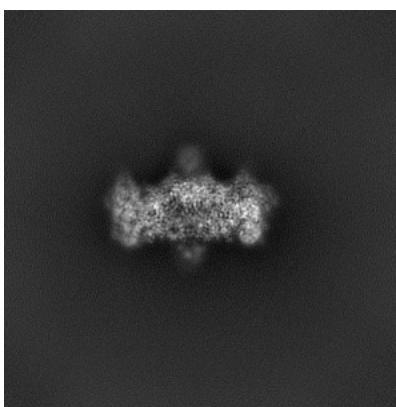


Z

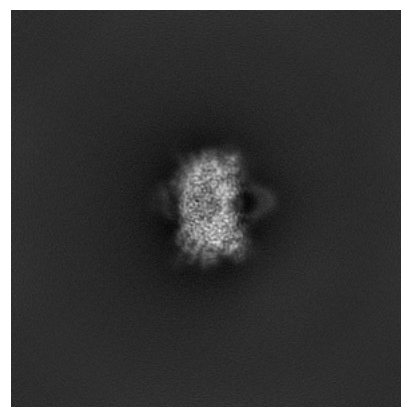
6.1.2 Raw map



X



Y

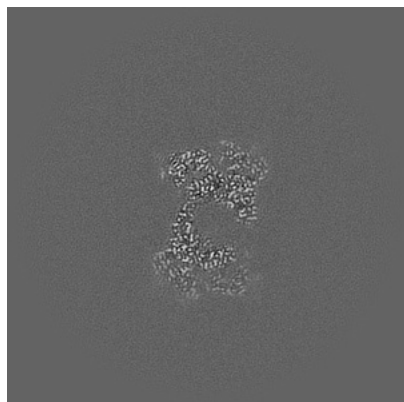


Z

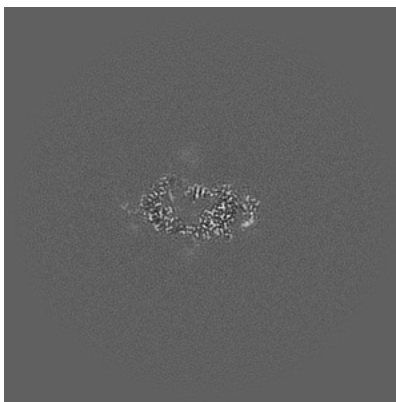
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

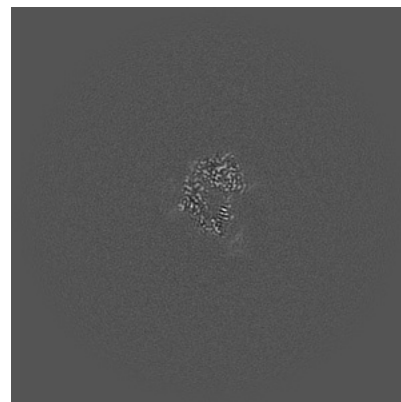
6.2.1 Primary map



X Index: 200

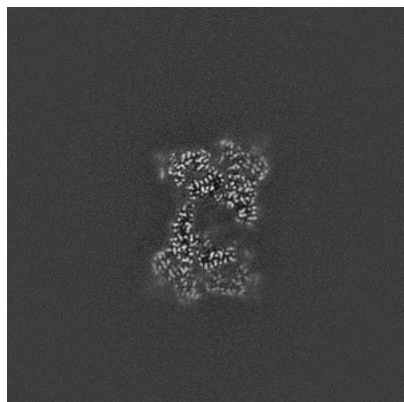


Y Index: 200

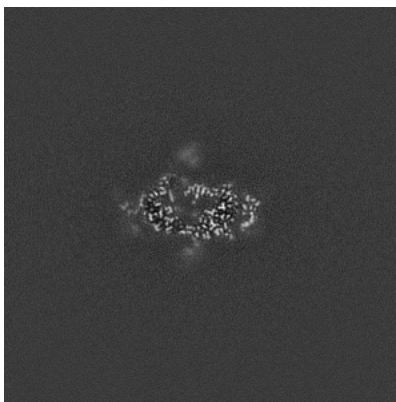


Z Index: 200

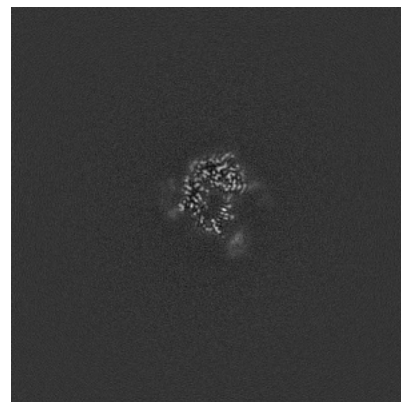
6.2.2 Raw map



X Index: 200



Y Index: 200

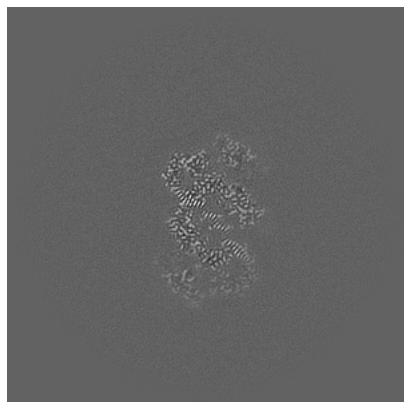


Z Index: 200

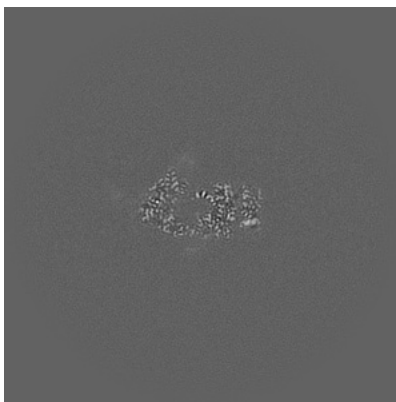
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

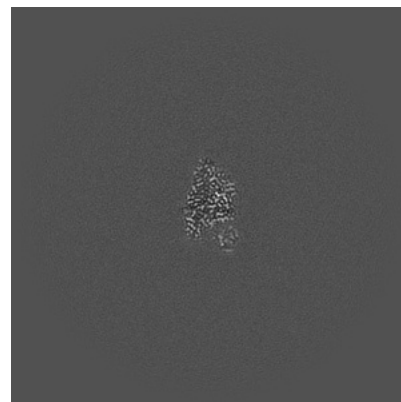
6.3.1 Primary map



X Index: 209

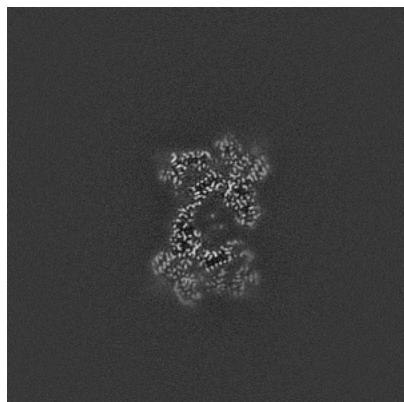


Y Index: 196

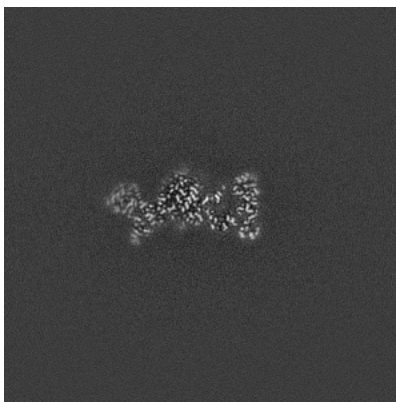


Z Index: 219

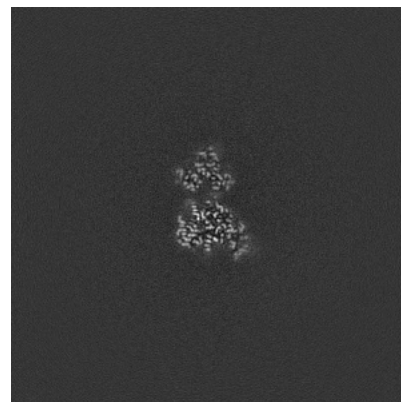
6.3.2 Raw map



X Index: 202



Y Index: 179

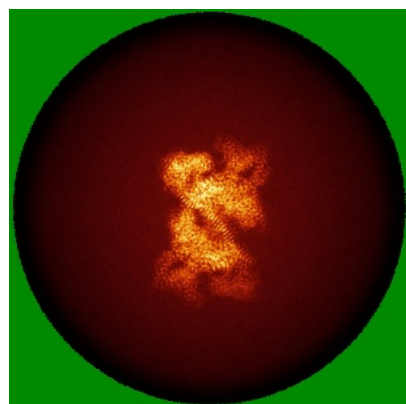


Z Index: 243

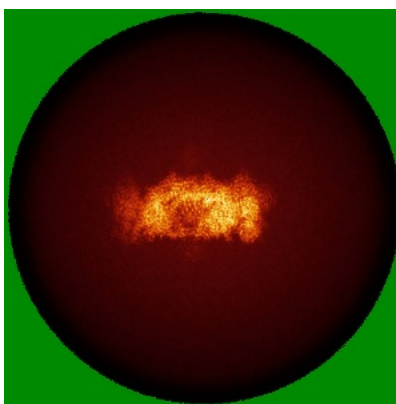
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

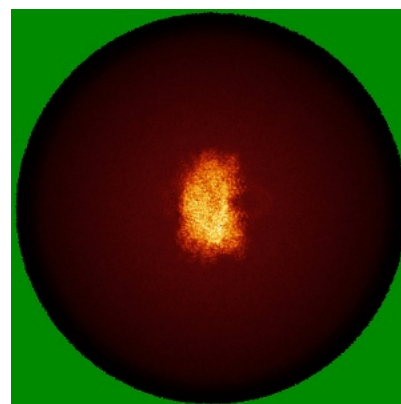
6.4.1 Primary map



X

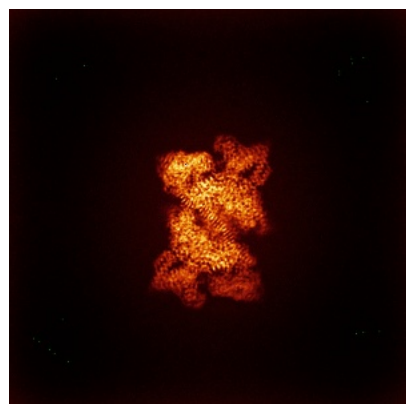


Y

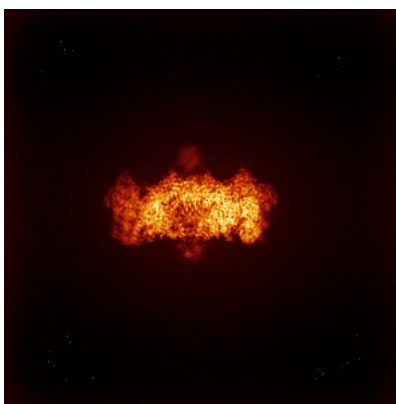


Z

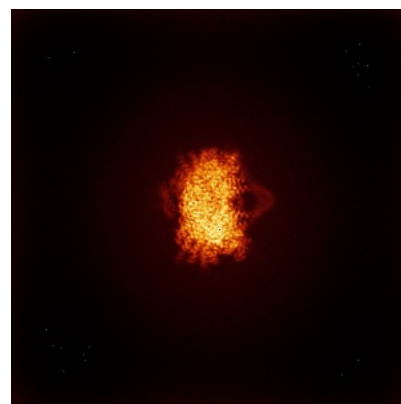
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

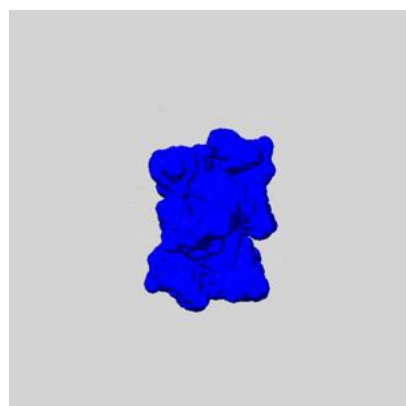
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

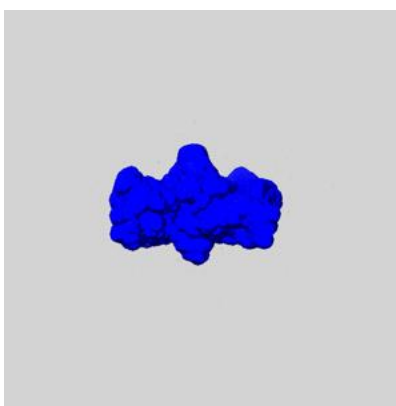
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

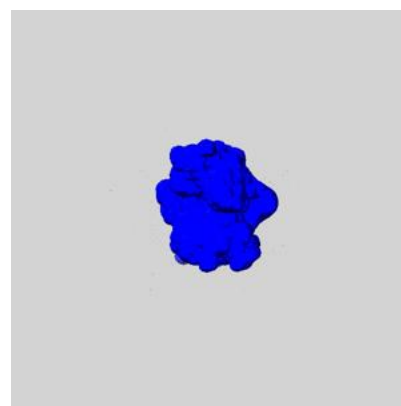
6.6.1 emd_62382_msk_1.map [i](#)



X



Y

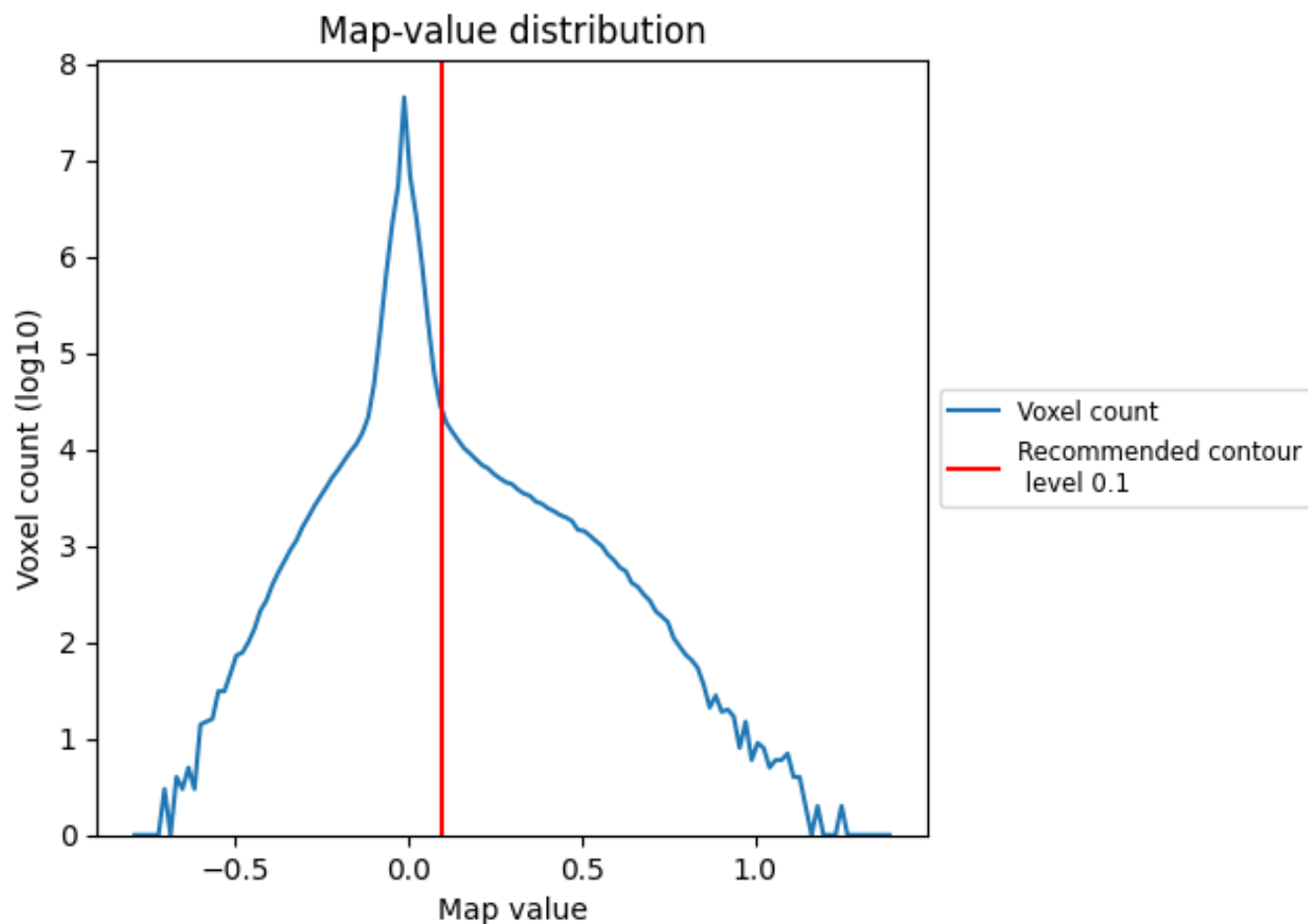


Z

7 Map analysis [i](#)

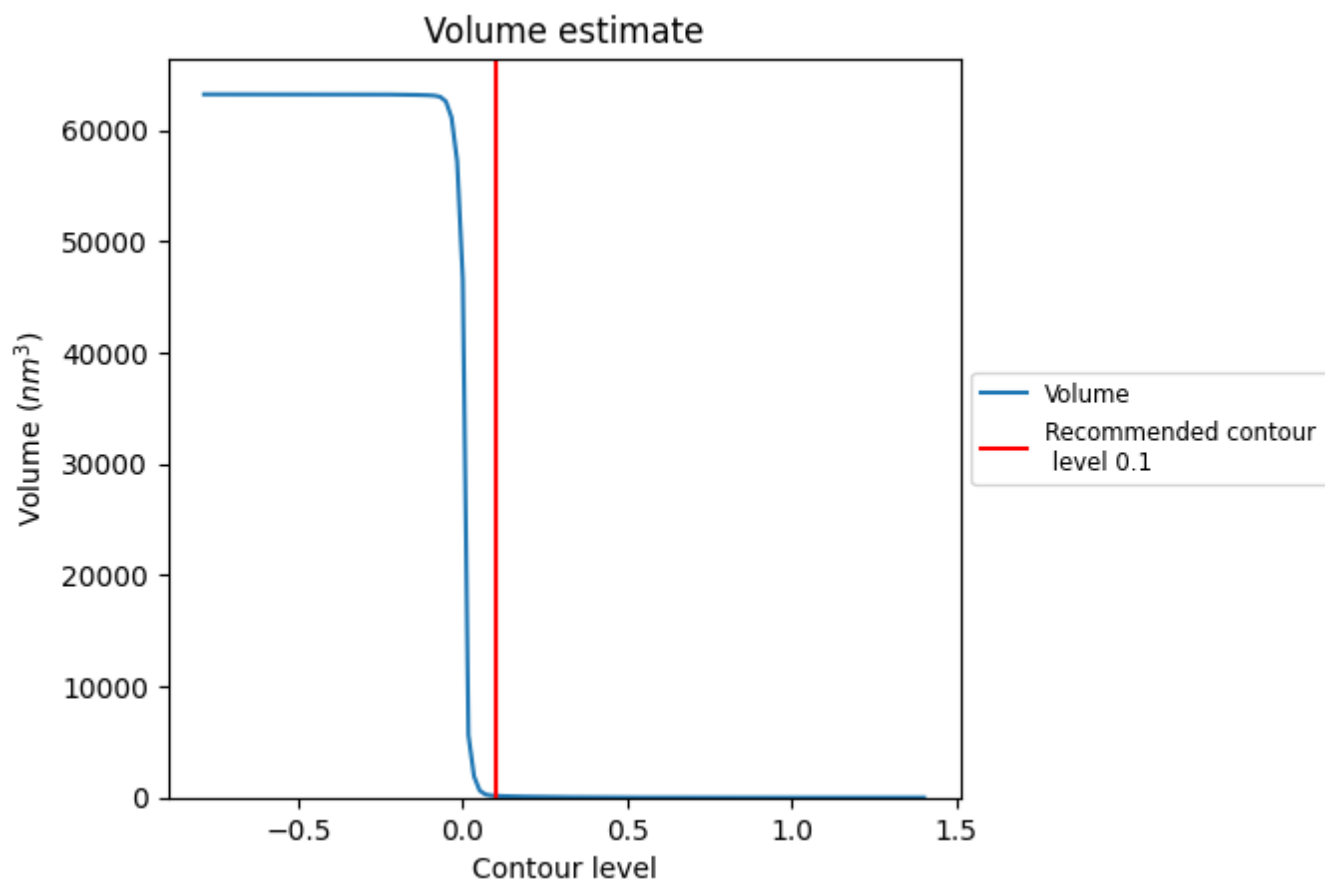
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

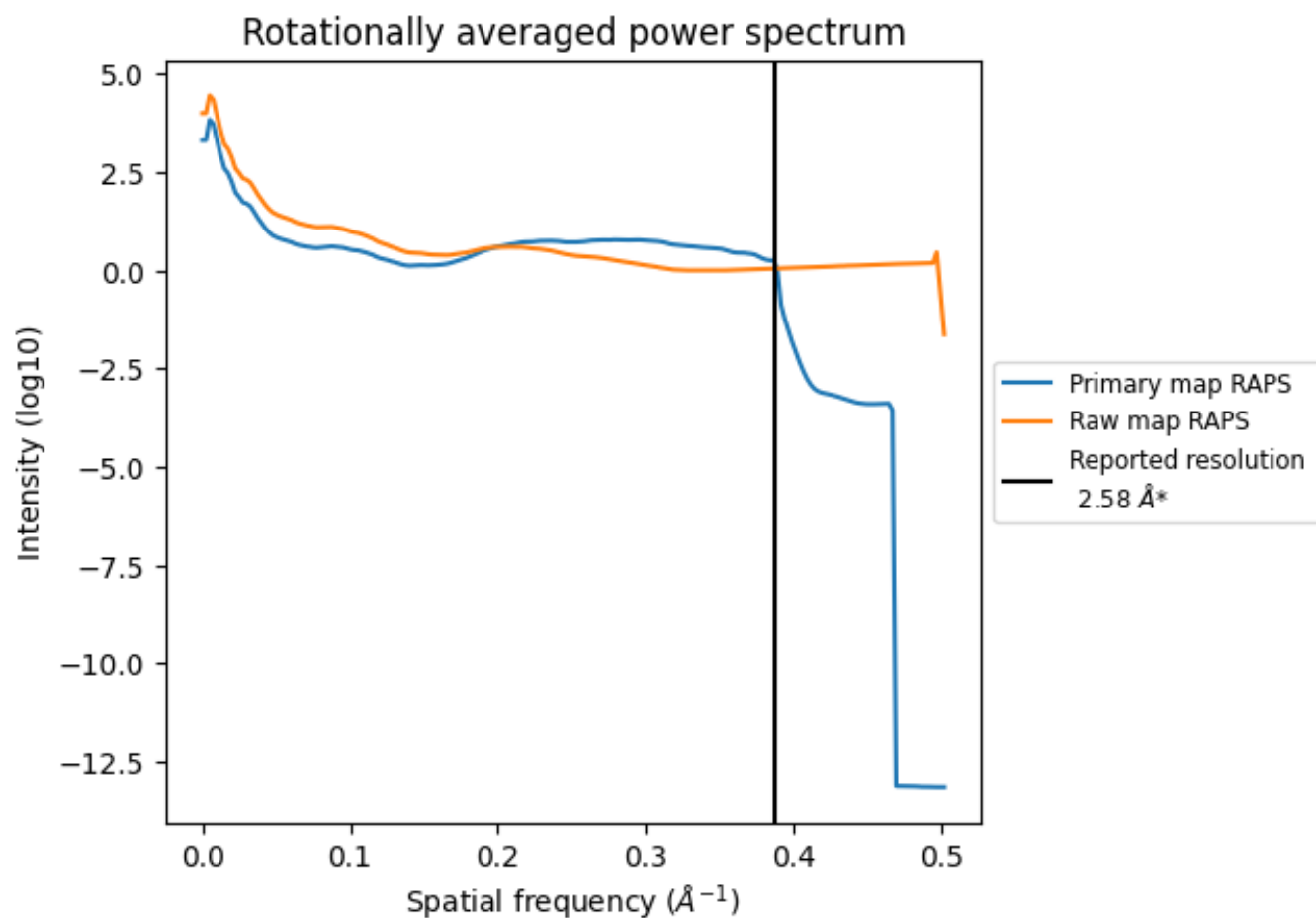
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm³; this corresponds to an approximate mass of 143 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

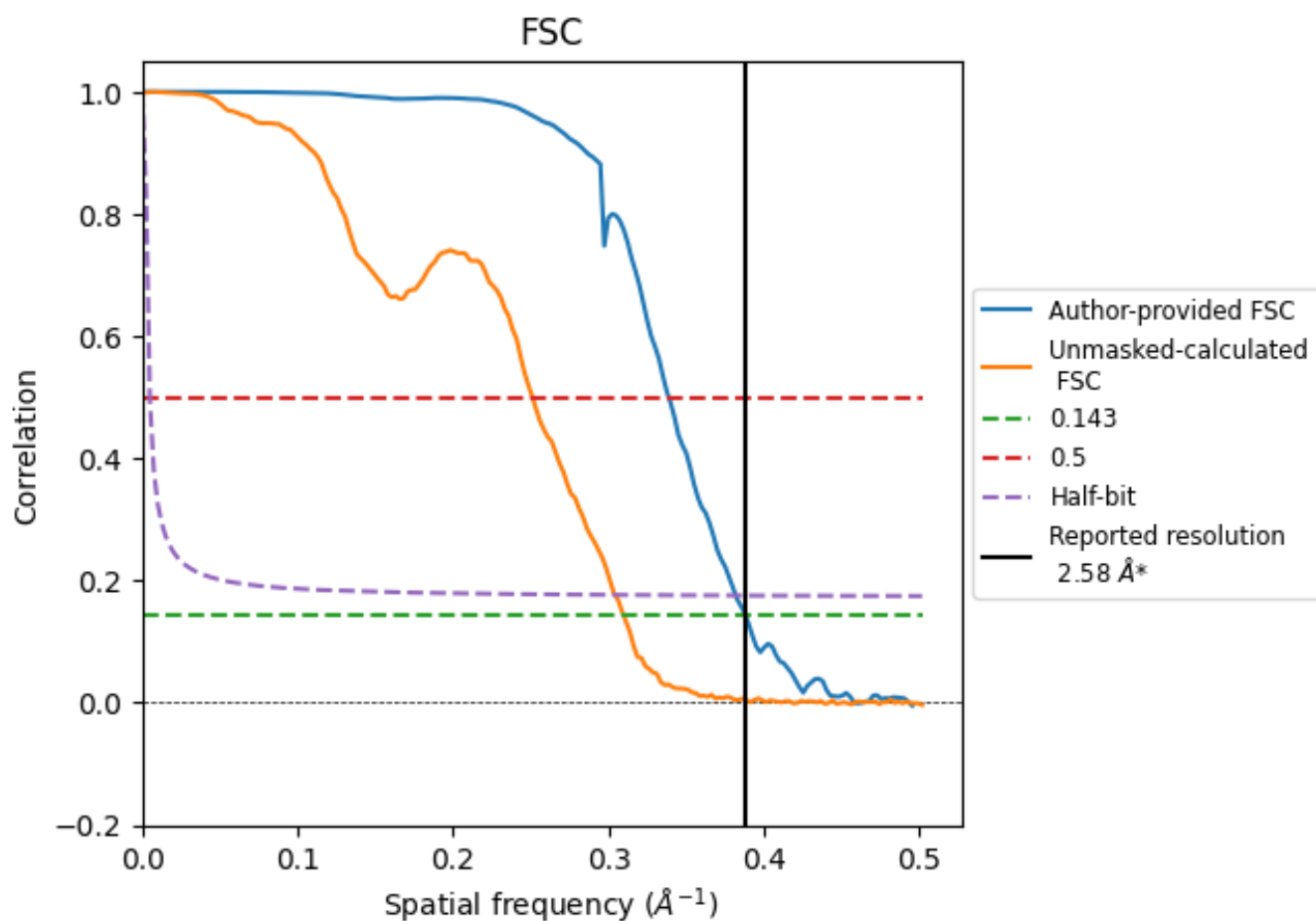


*Reported resolution corresponds to spatial frequency of 0.388 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

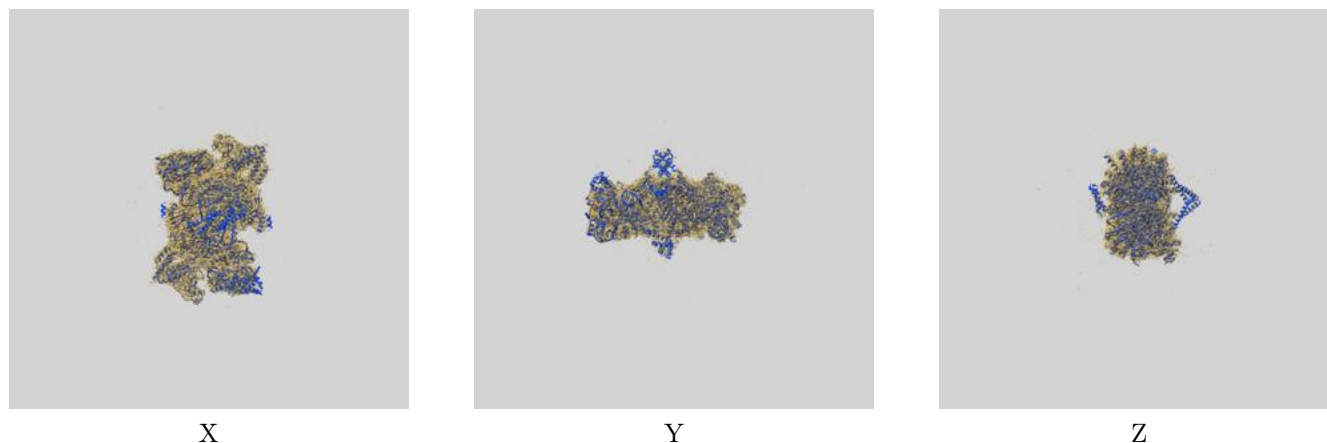
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.95	2.62
Unmasked-calculated*	3.23	3.98	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.58 by more than 10 %

9 Map-model fit [i](#)

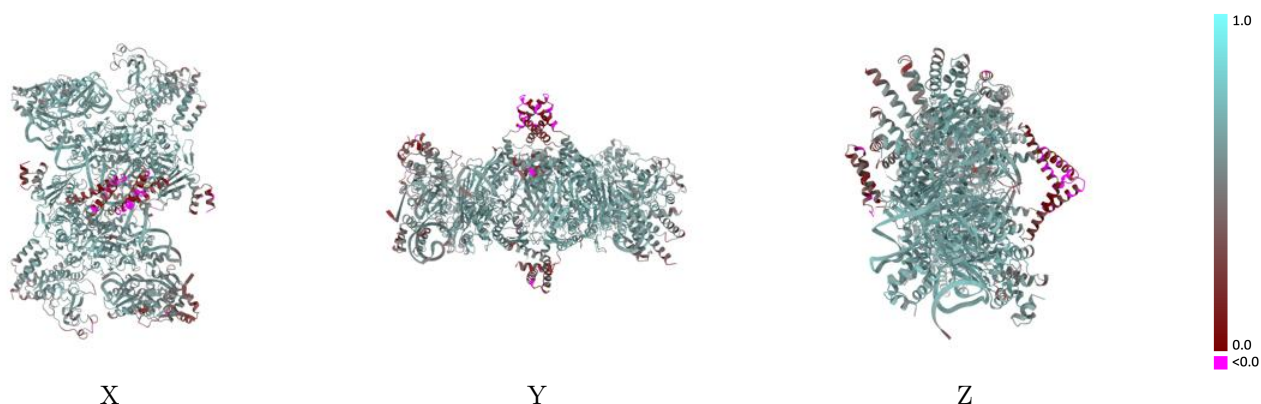
This section contains information regarding the fit between EMDB map EMD-62382 and PDB model 9KK2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

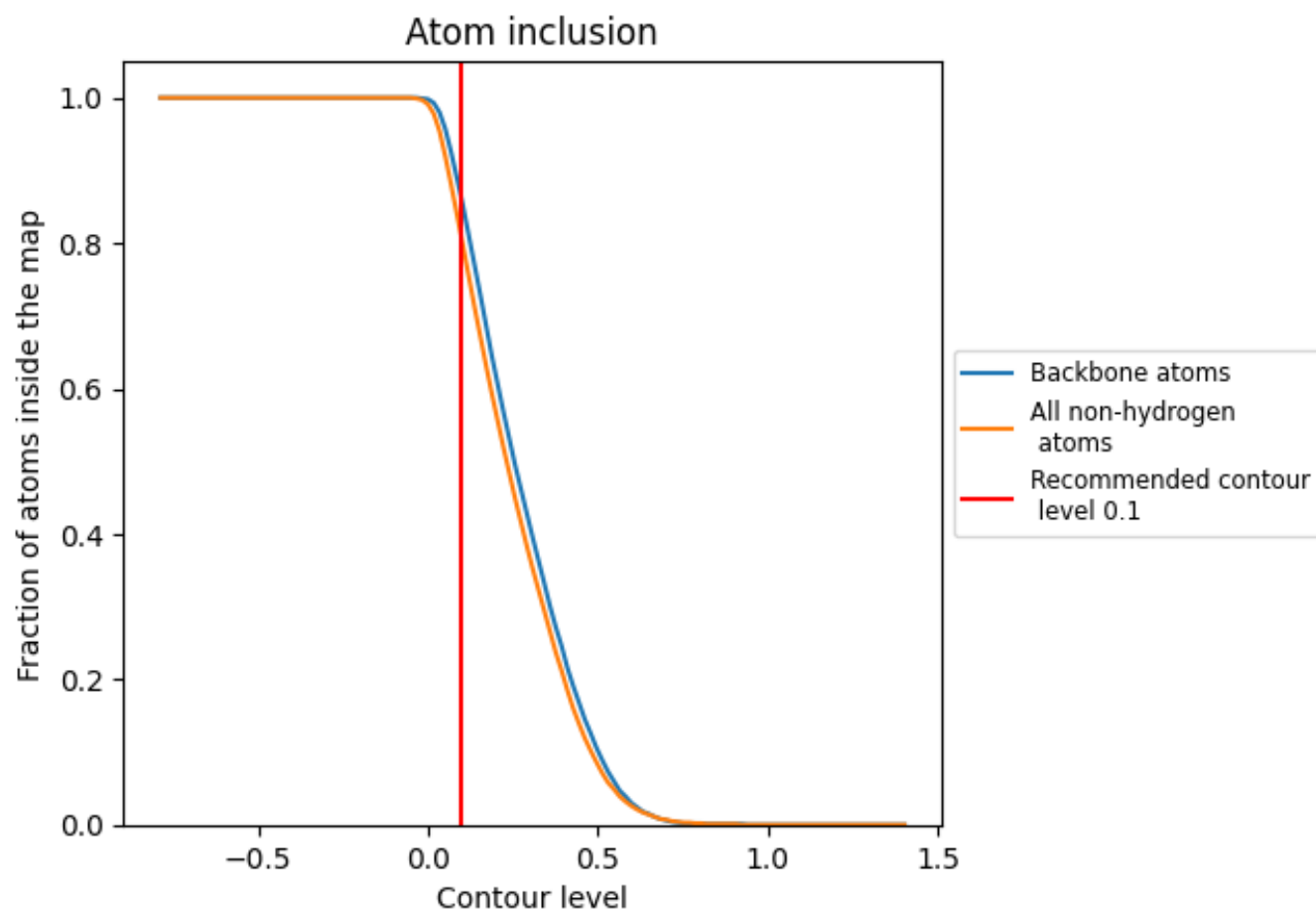


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.5760
A	0.9190	0.6300
B	0.8640	0.6080
C	0.7650	0.5400
D	0.7930	0.5660
E	0.8580	0.6030
F	0.8020	0.5620
G	0.7160	0.5290
H	0.9630	0.6380
I	0.9620	0.6360
K	0.5410	0.4980
L	0.7070	0.5520
M	0.6060	0.5360

1.0

0.0

<0.0